

## CHM 532

# Notes on Creation and Annihilation Operators

These notes provide the details concerning the solution to the quantum harmonic oscillator problem using the algebraic method discussed in class. The operators we introduce are called creation and annihilation operators, names that are taken from the quantum treatment of light (i.e. photons). The quantum treatment of electromagnetic radiation has similarities with the harmonic oscillator problem. In the study of photons, creation operators “create” photons and annihilation operators “annihilate” photons. As discussed below, creation operators “create” one quantum of energy in the harmonic oscillator and annihilation operators “annihilate” one quantum of energy.

We begin with the Hamiltonian operator for the harmonic oscillator expressed in terms of momentum and position operators taken to be independent of any particular representation

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2\hat{x}^2. \quad (1)$$

We next introduce the dimensionless operators  $\hat{Q}$  and  $\hat{P}$ , related to  $\hat{x}$  and  $\hat{p}$  by the equations

$$\hat{x} = \left(\frac{\hbar}{\mu\omega}\right)^{1/2} \hat{Q} \quad (2)$$

and

$$\hat{p} = (\mu\omega\hbar)^{1/2} \hat{P}. \quad (3)$$

Using

$$[\hat{x}, \hat{p}] = i\hbar \quad (4)$$

it can easily be shown that

$$[\hat{Q}, \hat{P}] = i. \quad (5)$$

Substituting Eqs. (2) and (3) into Eq.(1) we obtain

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{P}^2 + \hat{Q}^2). \quad (6)$$

We next define

$$\hat{H}_1 = \frac{\hat{H}}{\hbar\omega} = \frac{1}{2}(\hat{P}^2 + \hat{Q}^2). \quad (7)$$

It is easy to see that if  $\psi$  is an eigenfunction of  $\hat{H}_1$  with the dimensionless eigenvalue  $\epsilon$ , then  $\psi$  is also an eigenfunction of  $\hat{H}$  with eigenvalue  $E = \hbar\omega\epsilon$ .

We next define an *annihilation operator* by

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{Q} + i\hat{P}). \quad (8)$$

The adjoint of the annihilation operator

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{Q} - i\hat{P}) \quad (9)$$

is called a *creation operator*. Clearly,  $\hat{a}$  is not Hermitian. Using Eq.(5), it is easy to show that the commutator between creation and annihilation operators is given by

$$[\hat{a}, \hat{a}^\dagger] = 1. \quad (10)$$

We next solve Eqs.(8) and (9) for  $\hat{Q}$  and  $\hat{P}$

$$\hat{Q} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger) \quad (11)$$

$$\hat{P} = \frac{1}{i\sqrt{2}}(\hat{a} - \hat{a}^\dagger) \quad (12)$$

and substitute into Eq.(7) to obtain

$$\hat{H}_1 = \frac{1}{2} \left( \frac{1}{2}(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) - \frac{1}{2}(\hat{a}^2 + \hat{a}^{\dagger 2} - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}) \right) \quad (13)$$

$$= \frac{1}{2}(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}). \quad (14)$$

Using the commutator Eq.(10), the expression for  $\hat{H}_1$  becomes

$$\hat{H}_1 = \frac{1}{2}(2\hat{a}^\dagger\hat{a} + 1) = \hat{N} + \frac{1}{2}, \quad (15)$$

where

$$\hat{N} = \hat{a}^\dagger\hat{a} \quad (16)$$

is called the *number operator*. We see that if  $\psi_n$  is an eigenfunction function of  $\hat{N}$  with eigenvalue  $n$ ; i.e.

$$\hat{N}\psi_n = n\psi_n \quad (17)$$

then  $\psi_n$  is also an eigenfunction of  $\hat{H}_1$  with eigenvalue  $n + 1/2$  as well as an eigenfunction of  $\hat{H}$  with eigenvalue  $(n + 1/2)\hbar\omega$ . We seek then the eigenfunctions and eigenvalues of  $\hat{N}$ .

We begin with Eq.(17), and we assume the eigenfunctions have been normalized so that

$$\langle \psi_n | \psi_m \rangle = \delta_{n,m}. \quad (18)$$

We derive the eigenvalues of  $\hat{N}$  by proving a series of lemmas. The proofs of the lemmas make use of Eq.(10).

**Lemma 1**

$$n \geq 0. \quad (19)$$

Proof:

$$n = \langle \psi_n | \hat{N} | \psi_n \rangle \quad (20)$$

$$= \langle \psi_n | \hat{a}^\dagger \hat{a} | \psi_n \rangle \quad (21)$$

$$= \langle \hat{a} \psi_n | \hat{a} \psi_n \rangle \geq 0 \quad (22)$$

□

**Lemma 2**

$$\hat{N} \hat{a} = \hat{a} (\hat{N} - 1). \quad (23)$$

Proof:

$$\hat{N} \hat{a} = \hat{a}^\dagger \hat{a} \hat{a} \quad (24)$$

$$= (\hat{a} \hat{a}^\dagger - 1) \hat{a} \quad (25)$$

$$= \hat{a} (\hat{a}^\dagger \hat{a} - 1) = \hat{a} (\hat{N} - 1). \quad (26)$$

□

**Lemma 3**

$$\hat{N} \hat{a}^\dagger = \hat{a}^\dagger (\hat{N} + 1). \quad (27)$$

Proof:

$$\hat{N} \hat{a}^\dagger = \hat{a}^\dagger \hat{a} \hat{a}^\dagger \quad (28)$$

$$= \hat{a}^\dagger (\hat{a}^\dagger \hat{a} + 1) = \hat{a}^\dagger (\hat{N} + 1). \quad (29)$$

□

**Lemma 4**

$$\hat{a} \psi_n = c_- \psi_{n-1} \quad (30)$$

where  $c_-$  is a constant.

Proof:

We must show that  $\hat{a} \psi_n$  is an eigenfunction of  $\hat{N}$  with eigenvalue  $n - 1$ .

$$\hat{N} (\hat{a} \psi_n) = \hat{a} (\hat{N} - 1) \psi_n = \hat{a} (n - 1) \psi_n \quad (31)$$

$$= (n - 1) (\hat{a} \psi_n). \quad (32)$$

□

**Lemma 5**

$$\hat{a}^\dagger \psi_n = c_+ \psi_{n+1} \quad (33)$$

where  $c_+$  is a constant.

Proof:

We must show that  $\hat{a}^\dagger\psi_n$  is an eigenfunction of  $\hat{N}$  with eigenvalue  $n + 1$ .

$$\hat{N}(\hat{a}^\dagger\psi_n) = \hat{a}^\dagger(\hat{N} + 1)\psi_n = \hat{a}^\dagger(n + 1)\psi_n \quad (34)$$

$$= (n + 1)(\hat{a}^\dagger\psi_n). \quad (35)$$

□

**Lemma 6**

$$c_- = \sqrt{n} \quad (36)$$

and

$$c_+ = \sqrt{n + 1}. \quad (37)$$

Proof:

$$n = \langle \psi_n | \hat{N} | \psi_n \rangle = \langle \psi_n | \hat{a}^\dagger \hat{a} | \psi_n \rangle \quad (38)$$

$$= \langle \hat{a}\psi_n | \hat{a}\psi_n \rangle = c_-^2 \langle \psi_n | \psi_n \rangle = c_-^2 \quad (39)$$

or

$$c_- = \sqrt{n}. \quad (40)$$

Next

$$n + 1 = \langle \psi_n | \hat{N} + 1 | \psi_n \rangle = \langle \psi_n | \hat{a}^\dagger \hat{a} + 1 | \psi_n \rangle \quad (41)$$

$$= \langle \psi_n | \hat{a} \hat{a}^\dagger | \psi_n \rangle \quad (42)$$

$$= \langle \hat{a}^\dagger \psi_n | \hat{a}^\dagger \psi_n \rangle = c_+^2 \quad (43)$$

or

$$c_+ = \sqrt{n + 1}. \quad (44)$$

□

**Lemma 7**  $n$  is an integer.

Proof: We use the method of proof by contradiction. We assume  $n$  is not an integer, and show this leads to a result that contradicts one of our lemmas. We consider the process

$$\hat{a}\psi_n = \sqrt{n}\psi_{n-1} \quad (45)$$

$$\hat{a}^2\psi_n = \sqrt{n(n-1)}\psi_{n-2} \quad (46)$$

until

$$\hat{a}^m\psi_n = \sqrt{n(n-1)\dots(n-m+1)}\psi_{n-m}. \quad (47)$$

If  $n$  is not an integer, there exists a series of values of  $m$  such that  $n - m < 0$ . However, from the first lemma, the eigenvalue of  $\hat{N}$  must be positive or zero. Consequently, we have a contradiction, and  $n$  must be an integer.

□

**Lemma 8** *The smallest value of  $n$  is 0.*

Proof: Notice that

$$\hat{a}\psi_1 = \psi_0 \quad (48)$$

and

$$\hat{a}\psi_0 = 0. \quad (49)$$

Then  $n = 0$  is the smallest eigenvalue of  $\hat{N}$ .

□

We have then proved that the eigenvalues of  $\hat{N}$  are  $n = 0, 1, 2, \dots$ , and as a consequence, the eigenvalues of  $\hat{H}$  are  $E_n = (n + 1/2)\hbar\omega$  with  $n = 0, 1, 2, \dots$ , in agreement with the solution by differential equation. We next show that all matrix elements and expectation values of observables with respect to harmonic oscillator eigenfunctions can be evaluated using creation and annihilation operators. From Eqs.(2) and (11), we can write

$$\hat{x} = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (\hat{a} + \hat{a}^\dagger). \quad (50)$$

Then

$$\langle\psi_n|\hat{x}|\psi_m\rangle = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} \langle\psi_n|\hat{a} + \hat{a}^\dagger|\psi_m\rangle \quad (51)$$

$$= \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} \langle\psi_n|(\sqrt{m}|\psi_{m-1}\rangle + \sqrt{m+1}|\psi_{m+1}\rangle) \quad (52)$$

$$= \left(\frac{\hbar}{2\mu\omega}\right)^{1/2} (\sqrt{m}\delta_{n,m-1} + \sqrt{m+1}\delta_{n,m+1}). \quad (53)$$

The expectation value of  $x$  (i.e.  $n = m$ ) vanishes for any value of  $n$ . To evaluate matrix elements of  $\hat{x}^2$ , we use the operator

$$\hat{x}^2 = \frac{\hbar}{2\mu\omega} (\hat{a} + \hat{a}^\dagger)^2 \quad (54)$$

$$= \frac{\hbar}{2\mu\omega} (\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{N} + 1). \quad (55)$$

We end by showing that creation and annihilation operators can be used to construct the eigenfunctions of the Hamiltonian. We begin with the expression

$$\hat{a}\psi_0 = 0. \quad (56)$$

From Eq.(8), we have

$$\frac{1}{\sqrt{2}}(\hat{Q} + i\hat{P})\psi_0 = 0. \quad (57)$$

Now

$$\hat{P} = \left( \frac{1}{\mu\omega\hbar} \right)^{1/2} \hat{p} \quad (58)$$

$$= \left( \frac{1}{\mu\omega\hbar} \right)^{1/2} \frac{\hbar}{i} \frac{d}{dx} = \left( \frac{1}{\mu\omega\hbar} \right)^{1/2} \frac{\hbar}{i} \frac{dQ}{dx} \frac{d}{dQ} \quad (59)$$

$$\left( \frac{1}{\mu\omega\hbar} \right)^{1/2} \frac{\hbar}{i} \left( \frac{\mu\omega}{\hbar} \right)^{1/2} \frac{d}{dQ} = \frac{1}{i} \frac{d}{dQ}. \quad (60)$$

Then from Eq.(57)

$$\frac{d\psi_0}{dQ} + Q\psi_0 = 0 \quad (61)$$

which is easily solved to give

$$\psi_0 = Ae^{-Q^2/2} \quad (62)$$

where  $A$  is a constant. Using Eq.(2),  $\psi_0$  can be expressed in terms of the coordinate  $x$  and subsequently normalized to determine  $A$ . To determine  $\psi_1$ , we use

$$\hat{a}^\dagger \psi_0 = \psi_1 = \frac{1}{\sqrt{2}} \left( Q - \frac{d}{dQ} \right) \psi_0 = A' Q e^{-Q^2/2} \quad (63)$$

where  $A'$  is a constant. Again, using Eq.(2),  $\psi_1$  can be expressed in terms of  $x$  and normalized. Finally, it is easy to show that

$$\psi_n = \frac{1}{\sqrt{n!}} \hat{a}^{\dagger n} \psi_0. \quad (64)$$